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STATE-SELECTIVE CHARGE EXCHANGE CROSS SECTIONS IN Be^{4+}+ H(1s) COLLISION

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Abstract. Charge exchange *nl* partial cross sections have been calculated for collision of Be^{4+} with ground state hydrogen using the 3-body classical trajectory Monte Carlo method and quasiclassical trajectory Monte Carlo method of Kirschbaum and Wilets. The cross sections have been obtained for projectile n=1, 2, 3, 4 and 5 states and for corresponding allowed l quantum numbers. Calculations are carried out in the impact energy range between 1 and 1000 keV/au. Our results are compared to existing previous results. We showed that the calculations by QTMC-KW model improve the calculated cross sections.

1. INTRODUCTION

Beryllium is typically considered as the armor material for Plasma Facing Components (PFCs) of fusion devices and it is the first wall of the International Thermonuclear Experimental Reactor (ITER) (see Pitts et al. 2011). The inelastic collision processes between Be^{q+} ions and H are particularly important when energetic neutral hydrogen is injected into the plasma for heating and diagnostic purposes (see Hackman et al. 1984). Therefore the accurate description and knowledge of these interactions are extremely important for fusion research. The state-selective cross sections for charge exchange in collision between Be and hydrogen atom has been studied in the past using different theoretical approaches such as; MOCC method (see Harel et al. 1998, 1997), AOCC method (see Fritsch et al. 1984), OEDM (see Errea et al. 1982, 1998) and GTDSE method (see Jorge et al. 2016). The quasiclassical trajectory Monte Carlo method of Kirschbaum and Wilets (QTMC-KW) model (see Kirschbaun et al. 1980) is one step further for a better description of the classical atomic collisions. For atoms, a necessary condition for stability is that the electrons are not allowed to collapse to the symmetry point, i.e., to the nucleus. The effective potential enforcing this condition is motivated by the Heisenberg uncertainty principle $rp \geq \xi_H \hbar$, where r and p are the distance and momentum of an electron with respect to a nucleus and ξ_H is constant. For the H atom, this condition is equivalent to the de Broglie description of the hydrogen atom.

In this work we present state selective charge exchange cross sections in collision between Be^{4+} and ground state hydrogen atom using the 3-body classical trajectory Monte Carlo method (CTMC) and quasiclassical trajectory Monte Carlo method of Kirschbaum and Wilets (QTMC-KW). Our results are compared to existing previous results.

2. THEORY

In the present work, the CTMC simulations were made in the three-body approximation. The three particles (p; projectile, e; electron, T; target) are characterized by their masses and charges. For the description of the interaction among the particles, Coulomb potential is used. Figure 1 shows the relative position vectors of the three-body collision system.

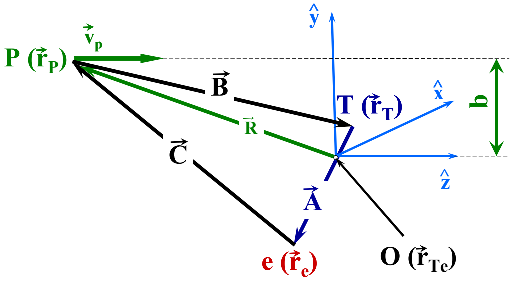

Figure 1: The relative position vectors of the particles involved in 3-body collisions. $\vec{A} = \vec{r}_e - \vec{r}_T$, $\vec{B} = \vec{r}_T - \vec{r}_p$ and $\vec{C} = \vec{r}_p - \vec{r}_e$, in such way that $\vec{A} + \vec{B} + \vec{C} = 0$. Also, $\vec{r}_{\mathrm{Te}}$ is the position vector of the center-of-mass of the target system, and b is the impact parameter.

For the more accurate classical simulation results, we must also consider the rule of Heisenberg and Pauli principles. This approach was proposed by Kirschbaum and Wilets (KW) as a fermion molecular dynamic model (FMD). According to this model the effective potential, V_H motivated by the Heisenberg principles, is added to the pure Coulomb inter-particle potentials describing the classical atom. Thus

$$H_{FMD} = H_0 + V_H \tag{1}$$

where H_0 is the usual Hamiltonian containing the total kinetic energy of all bodies and Coulomb potential terms between all pairs of electrons and between the nucleus and electrons, respectively. The extra term is

$$V_H = \sum_{n=a,b} \sum_{i=1}^{N} f\left(r_{ni}, p_{ni}; \xi_H, \alpha_H\right), \tag{2}$$

where a and b denote the nuclei and the i, j index the electrons. Also, $r_{\alpha\beta} = r_\beta - r_\alpha$ and relative momenta are:

$$p_{\alpha\beta} = \frac{m_\alpha p_\beta - m_\beta m_\alpha}{m_\alpha + m_\beta} \tag{3}$$

The constraining potential can be written in the following form

$$f\left(r_{\lambda\nu}, p_{\lambda\nu}; \xi, \alpha\right) = \frac{\xi}{4\alpha r_{\lambda\nu}^{2}\mu_{\lambda\nu}} exp\left\{\alpha\left[1-\left(\frac{r_{\lambda\nu}p_{\lambda\nu}}{\xi}\right)^{4}\right]\right\} \tag{4}$$

In this work, α_H=4 and ξ_H= 0.9428 are used in Eq. 4 for the description of the Heisenberg constrain, respectively.

3. RESULTS

To study the collision between Be^{4+} and hydrogen atom we used both the standard 3-body classical trajectory Monte Carlo (CTMC) and quasiclassical trajectory Monte Carlo method of Kirschbaum and Wilets (QTMC-KW) methods. We performed a classical simulation with an ensemble of 1×10^{6} primary trajectories for each energy. The calculations were carried out in the projectile energy range between 10 and 1000 keV/au, relevant to the interest of the fusion research when the target hydrogen atom is in the ground state. We estimate uncertainties in our calculation as 0.6% error. It is worth nothing that, this is the first time to present state–selective cross section data using the QTMC-KW method for Be^{4+} + H(1s) system.

The accurate knowledge of the charge exchange cross sections in fusion plasma is very important. For example, the charge exchange recombination spectroscopy (CXRS) measurements using Be^{4+} provide a high quality determination of the plasma parameters. The quality of such concentration measurements relies on the accuracy of the charge exchange cross sections. We have calculated the state-selective charge exchange cross section to the projectile bound state (see Eq. 5.) according to CTMC and QTMC-KW methods.

$$Be^{4+} + H(1s) \rightarrow Be^{3+}(nl) + H^{+} \tag{5}$$

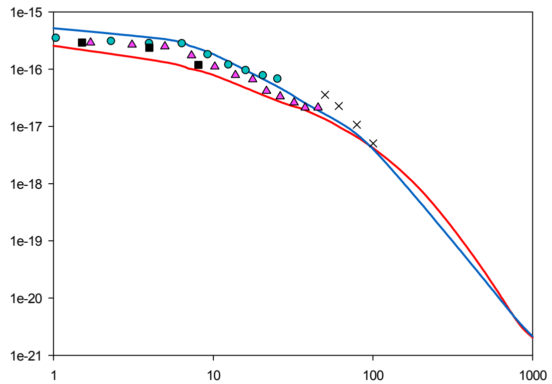

Figure 2 : State-selective charge exchange cross section into the 3s state of the projectile in Be^{4+} + H(1s) collision, as a function of the impact energy. CTMC (solid red line), QTMC-KW (solid blue line), MOCC (Harel) (●), AOCC (Fritsch) (■), OEDM (Errea) (▲), BCCIS (Das) (×).

Figure 2 shows the state-selective charge exchange cross section into the 3s state of the projectile in Be^{4+} + H(1s) collision. According to Fig 2., we found improvement in the cross section using QTMC-KW method compared to the standard CTMC model. We also found excellent agreement between our QTMC-KW results and the previous data.

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